

10/552,459

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NEWS	1		Web Page for STN Seminar Schedule - N. America
NEWS	2	MAY 01	New CAS web site launched
NEWS	3	MAY 08	CA/Capplus Indian patent publication number format defined
NEWS	4	MAY 14	RDISCLOSURE on STN Easy enhanced with new search and display fields
NEWS	5	MAY 21	BIOSIS reloaded and enhanced with archival data
NEWS	6	MAY 21	TOXCENTER enhanced with BIOSIS reload
NEWS	7	MAY 21	CA/Capplus enhanced with additional kind codes for German patents
NEWS	8	MAY 22	CA/Capplus enhanced with IPC reclassification in Japanese patents
NEWS	9	JUN 27	CA/Capplus enhanced with pre-1967 CAS Registry Numbers
NEWS	10	JUN 29	STN Viewer now available
NEWS	11	JUN 29	STN Express, Version 8.2, now available
NEWS	12	JUL 02	LEMBASE coverage updated
NEWS	13	JUL 02	LMEDLINE coverage updated
NEWS	14	JUL 02	SCISEARCH enhanced with complete author names
NEWS	15	JUL 02	CHEMCATS accession numbers revised
NEWS	16	JUL 02	CA/Capplus enhanced with utility model patents from China
NEWS	17	JUL 16	Capplus enhanced with French and German abstracts
NEWS	18	JUL 18	CA/Capplus patent coverage enhanced
NEWS	19	JUL 26	USPATFULL/USPAT2 enhanced with IPC reclassification
NEWS	20	JUL 30	USGENE now available on STN
NEWS	21	AUG 06	CAS REGISTRY enhanced with new experimental property tags
NEWS	22	AUG 06	BEILSTEIN updated with new compounds
NEWS	23	AUG 06	FSTA enhanced with new thesaurus edition
NEWS	24	AUG 13	CA/Capplus enhanced with additional kind codes for granted patents
NEWS	25	AUG 20	CA/Capplus enhanced with CAS indexing in pre-1907 records
NEWS	26	AUG 27	Full-text patent databases enhanced with predefined patent family display formats from INPADOCDB
NEWS	27	AUG 27	USPATOLD now available on STN
NEWS	28	AUG 28	CAS REGISTRY enhanced with additional experimental spectral property data

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NEWS EXPRESS 29 JUNE 2007: CURRENT WINDOWS VERSION IS V8.2,
CURRENT MACINTOSH VERSION IS V6.0c(ENG) AND V6.0Jc(JP),
AND CURRENT DISCOVER FILE IS DATED 05 JULY 2007.

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FILE 'HOME' ENTERED AT 17:47:16 ON 02 SEP 2007

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ENTRY	SESSION
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FULL ESTIMATED COST

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STRUCTURE FILE UPDATES: 31 AUG 2007 HIGHEST RN 945948-91-4

DICTIONARY FILE UPDATES: 31 AUG 2007 HIGHEST RN 945948-91-4

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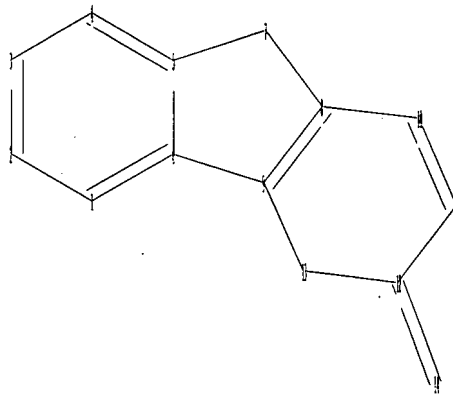
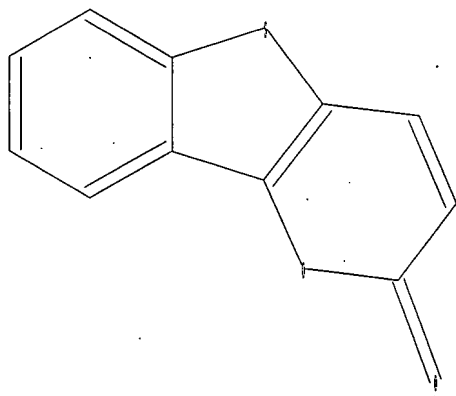
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<http://www.cas.org/support/stngen/stndoc/properties.html>

=>

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Uploading C:\Program Files\Stnexp\Queries\10552459.str



chain nodes :

14

ring nodes :

1 2 3 4 5 6 7 8 9 10 11 12 13

chain bonds :

12-14

ring bonds :

1-2 1-6 2-3 3-4 4-5 5-6 5-7 6-9 7-8 8-9 8-10 9-13 10-11 11-12

12-13

exact/norm bonds :

12-14

exact bonds :

5-7 6-9 7-8 8-9 8-10 9-13 10-11 11-12 12-13

normalized bonds :

1-2 1-6 2-3 3-4 4-5 5-6

isolated ring systems :

containing 1 :

Match level :

1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:Atom 8:Atom 9:Atom

10:Atom 11:Atom 12:Atom 13:Atom 14:CLASS

L1 STRUCTURE UPLOADED

=> s l1

SAMPLE SEARCH INITIATED 17:47:54 FILE 'REGISTRY'

SAMPLE SCREEN SEARCH COMPLETED - 1 TO ITERATE

100.0% PROCESSED 1 ITERATIONS

1 ANSWERS

SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS: ONLINE **COMPLETE**
BATCH **COMPLETE**

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PROJECTED ITERATIONS: 1 TO 80
PROJECTED ANSWERS: 1 TO 80

L2 1 SEA SSS SAM L1

=> s l1 ful

FULL SEARCH INITIATED 17:48:02 FILE 'REGISTRY'
FULL SCREEN SEARCH COMPLETED - 56 TO ITERATE

100.0% PROCESSED 56 ITERATIONS 52 ANSWERS
SEARCH TIME: 00.00.01

L3 52 SEA SSS FUL L1

=> file caplus

COST IN U.S. DOLLARS	SINCE FILE ENTRY	TOTAL SESSION
FULL ESTIMATED COST	172.10	172.31

FILE 'CAPLUS' ENTERED AT 17:48:12 ON 02 SEP 2007
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FILE LAST UPDATED: 31 Aug 2007 (20070831/ED)

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<http://www.cas.org/infopolicy.html>

=> s l3

L4 16 L3

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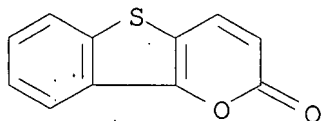
L4 ANSWER 1 OF 16 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 2004:902391 CAPLUS
DOCUMENT NUMBER: 141:370267
TITLE: Fragrance compositions comprising
benzo[4,5]thieno[3,2-

10/552,459

INVENTOR(S): b]pyran-2-one
Turin, Luca
PATENT ASSIGNEE(S): Flexitral, Inc., USA
SOURCE: PCT Int. Appl., 28 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2004092182	A1	20041028	WO 2004-US10829	20040408
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NA, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW				
RW: BW, GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG				
AU 2004230923	A1	20041028	AU 2004-230923	20040408
CA 2521834	A1	20041028	CA 2004-2521834	20040408
EP 1622915	A1	20060208	EP 2004-759279	20040408
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, FI, RO, CY, TR, BG, CZ, EE, HU, PL, SK				
GB 2418915	A	20060412	GB 2005-22412	20040408
CN 1784411	A	20060607	CN 2004-80012014	20040408
JP 2006526623	T	20061124	JP 2006-509812	20040408
US 2006292097	A1	20061228	US 2006-552459 ✓	20060804
PRIORITY APPLN. INFO.:			US 2003-461090P	P 20030408
			WO 2004-US10829	W 20040408

IT 5732-22-9P, Tonkené
RL: COS (Cosmetic use); FFD (Food or feed use); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(preparation of aromachems. for fragrances and flavorings)
RN 5732-22-9 CAPLUS
CN 2H-[1]Benzothieno[3,2-b]pyran-2-one (8CI, 9CI) (CA INDEX NAME)



10/552,459

AB The present invention relates to perfumes and other fragrant articles based on aromachems. which overcome the stability limitations and/or allergenic nature of the native compds. Particularly, compns. comprising at least 30% of benzo[4,5]thieno[3,2-b]pyran-2-one employed as aroma chemical for fragrances and flavorings are described. For example, benzo[4,5]thieno[3,2-b]pyran-2-one was synthesized by reacting 2-mercaptobenzoic acid with trans-glutaconic acid in the presence of a catalytic amount of sulfuric acid.

REFERENCE COUNT: 2 THERE ARE 2 CITED REFERENCES AVAILABLE FOR THIS

FORMAT RECORD. ALL CITATIONS AVAILABLE IN THE RE

=> d 14 ibib hitstr abs 2-16

L4 ANSWER 2 OF 16 CAPLUS COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER: 1998:351145 CAPLUS

DOCUMENT NUMBER: 129:31781

TITLE: Biodegradation of dibenzothiophene by a nodulating isolate of Rhizobium meliloti

AUTHOR(S): Frassinetti, Stefania; Setti, Leonardo; Corti, Andrea;

Farrinelli, Paolo; Montevocchi, Piercarlo; Vallini, Giovanni

CORPORATE SOURCE: National Research Council (CNR), Soil Microbiology Center, Pisa, 56124, Italy

SOURCE: Canadian Journal of Microbiology (1998), 44(3), 289-297

CODEN: CJMIAZ; ISSN: 0008-4166

PUBLISHER: National Research Council of Canada

DOCUMENT TYPE: Journal

LANGUAGE: English

IT 5732-22-9, 2H-[1]Benzothieno[3,2-b]pyran-2-one

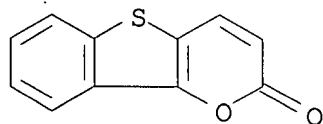
RL: BPR (Biological process); BSU (Biological study, unclassified); MFM (Metabolic formation); REM (Removal or disposal); BIOL (Biological study);

FORM (Formation, nonpreparative); PROC (Process)

(formation of; in biodegrdn. of dibenzothiophene by a nodulating isolate of Rhizobium meliloti).

RN 5732-22-9 CAPLUS

CN 2H-[1]Benzothieno[3,2-b]pyran-2-one (8CI, 9CI) (CA INDEX NAME)



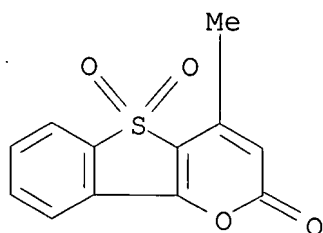
10/552,459

AB Rhizobium meliloti strain Orange 1 was isolated from aerobic sediments
of a drainage ditch receiving oil refinery leakage. This bacterium has
been shown to be capable of growing on dibenzothiophene as the sole carbon
and energy source. This strain can also efficaciously nodulate alfalfa
plants. In cultures with dibenzothiophene, strain Orange 1 produces
six degradation intermediates. By means of analyses with UV-visible
spectrometry and gas chromatog.-mass spectrometry, as well as NMR spectroscopy,
three of these products were identified as 3-hydroxy-2-formyl-benzothiophene
(product A), benzothienopyran-2-one (product B'), and
dibenzothiophene-5-oxide (product D). This suggests that R. meliloti strain Orange 1
metabolizes dibenzothiophene via oxidative cleavage of the aromatic
ring with a mechanism analogous to that described for naphthalene degradation
REFERENCE COUNT: 35 THERE ARE 35 CITED REFERENCES AVAILABLE FOR
THIS

RECORD. ALL CITATIONS AVAILABLE IN THE RE
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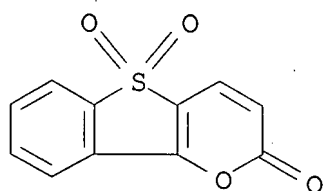
L4 ANSWER 3 OF 16 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 1989:154182 CAPLUS
DOCUMENT NUMBER: 110:154182
TITLE: Some reactions of
2H-[1]benzothieno[3,2-b]pyran-2-ones
and related compounds
AUTHOR(S): Buggle, Katherine; Ghogain, Una Ni; MacManus,
Patrick
CORPORATE SOURCE: Dep. Chem., Univ. Coll., Dublin, Ire.
SOURCE: Monatshefte fuer Chemie (1988), 119(8-9), 945-51
CODEN: MOCMB7; ISSN: 0026-9247
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 110:154182
IT 119872-67-2P 119872-68-3P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation);
RACT (Reactant or reagent)
(preparation and thiation of)
RN 119872-67-2 CAPLUS
CN 2H-[1]Benzothieno[3,2-b]pyran-2-one, 4-methyl-, 5,5-dioxide (9CI) (CA
INDEX NAME)

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RN 119872-68-3 CAPLUS

CN 2H-[1]Benzothieno[3,2-b]pyran-2-one, 5,5-dioxide (9CI) (CA INDEX NAME)

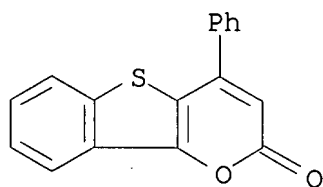


IT 87894-69-7

RL: RCT (Reactant); RACT (Reactant or reagent)
(reaction with acetylenedicarboxylate)

RN 87894-69-7 CAPLUS

CN 2H-[1]Benzothieno[3,2-b]pyran-2-one, 4-phenyl- (9CI) (CA INDEX NAME)

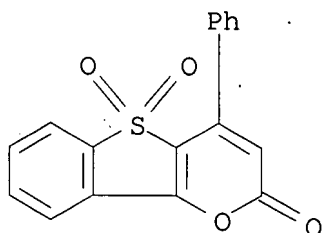


IT 87894-70-0

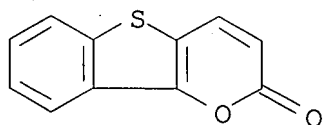
RL: RCT (Reactant); RACT (Reactant or reagent)
(thiation or reaction with methylamine)

RN 87894-70-0 CAPLUS

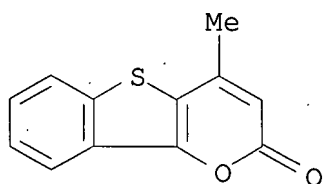
CN 2H-[1]Benzothieno[3,2-b]pyran-2-one, 4-phenyl-, 5,5-dioxide (9CI) (CA INDEX NAME)



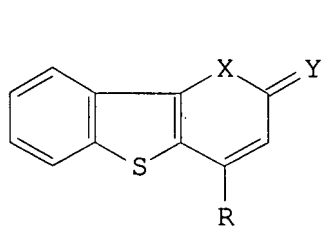
IT 5732-22-9, 2H-[1]Benzothieno[3,2-b]pyran-2-one 119872-66-1
 RL: RCT (Reactant); RACT (Reactant or reagent)
 (S-oxidation and thiation of)
 RN 5732-22-9 CAPLUS
 CN 2H-[1]Benzothieno[3,2-b]pyran-2-one (8CI, 9CI) (CA INDEX NAME)



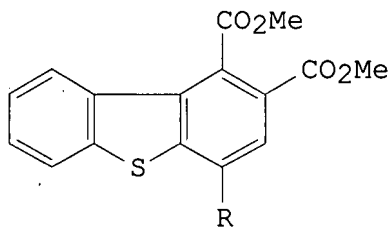
RN 119872-66-1 CAPLUS
 CN 2H-[1]Benzothieno[3,2-b]pyran-2-one, 4-methyl- (9CI) (CA INDEX NAME)



GI



I



II

AB The conversion of 2H-[1]benzothieno[3,2-b]pyran-2-ones I (X = Y = O, R = Ph, Me, H) into mono- and dithio derivs. and the preparation of some dibenzothiophenes (II) sulfines I (X = S, Y = SO) and pyridones I (X =

10/552,459

NMe, Y = O) are described.

L4 ANSWER 4 OF 16 CAPLUS COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER: 1984:120920 CAPLUS

DOCUMENT NUMBER: 100:120920

TITLE: Annelation of the 2-aminopyran-4-one ring to
condensed

thiophenes

AUTHOR(S): Volovenko, Yu. M.; Litenko, V. A.; Khrapak, T. V.;
Babichev, F. S.

CORPORATE SOURCE: Kiev. Gos. Univ., Kiev, 252017, USSR

SOURCE: Khimiya Geterotsiklicheskikh Soedinenii. (1983),
(11),

1476-8

CODEN: KGSSAQ; ISSN: 0453-8234

DOCUMENT TYPE: Journal

LANGUAGE: Russian

OTHER SOURCE(S): CASREACT 100:120920

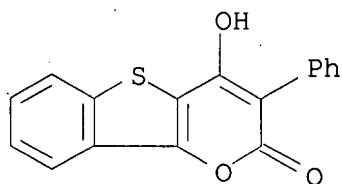
IT 89155-19-1P

RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)

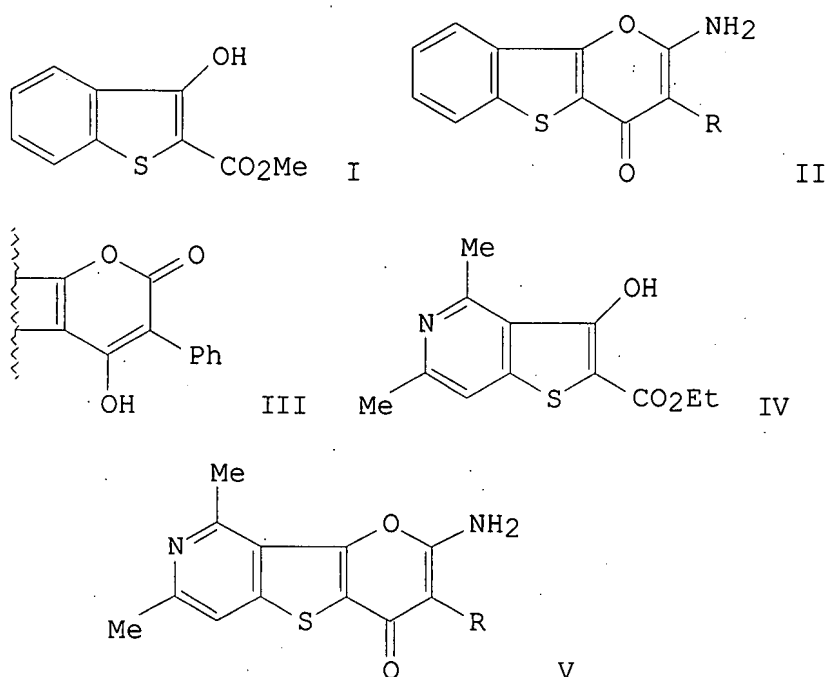
RN 89155-19-1 CAPLUS

CN 2H-[1]Benzothieno[3,2-b]pyran-2-one, 4-hydroxy-3-phenyl- (9CI) (CA
INDEX

NAME)



GI



AB Cyclocondensation of benzothiophenecarboxylate I with RCH_2CN [$\text{R} = \text{Ph}$, 2- ClC_6H_4 , 2,3,4-(MeO) $3\text{C}_6\text{H}_2$] catalyzed by Me_2CHONa gave 55-70% II which (R = Ph) was acetylated to give the N-acetyl derivative and hydrolyzed to give 70% III. Similar treatment of thienopyridinecarboxylate IV by RCH_2CN [R = Ph, 2- ClC_6H_4 , 3,4-(MeO) $2\text{C}_6\text{H}_3$] gave 83-90% V.

L4 ANSWER 5 OF 16 CAPLUS COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER: 1983:612429 CAPLUS

DOCUMENT NUMBER: 99:212429

TITLE: Thiopyrano[1]benzothiophenes. Synthesis of 1-phenyl-3H-thiopyrano[3,4-b][1]benzothiophene-3-thione 9,9-dioxide and related compounds

AUTHOR(S): Buggle, Katherine; Ghogain, Una Ni; Nangle, Michael;

MacManus, Patrick

CORPORATE SOURCE: Dep. Chem., Univ. Coll., Dublin, Ire.

SOURCE: Journal of the Chemical Society, Perkin Transactions

1: Organic and Bio-Organic Chemistry (1972-1999) (1983), (7), 1427-9

CODEN: JCPRB4; ISSN: 0300-922X

DOCUMENT TYPE: Journal

LANGUAGE: English

OTHER SOURCE(S): CASREACT 99:212429

10/552,459

IT 87894-69-7P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation);

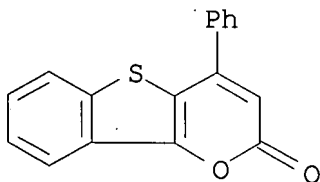
RACT

(Reactant or reagent)

(preparation and oxidation of)

RN 87894-69-7 CAPLUS

CN 2H-[1]Benzothieno[3,2-b]pyran-2-one, 4-phenyl- (9CI) (CA INDEX NAME)



IT 87894-70-0P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation);

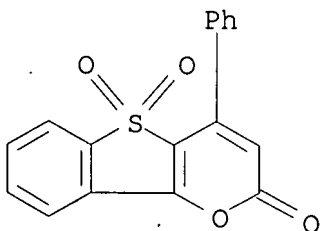
RACT

(Reactant or reagent)

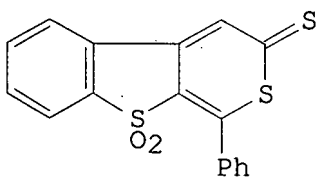
(preparation and sulfuration of)

RN 87894-70-0 CAPLUS

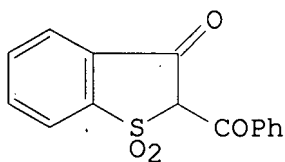
CN 2H-[1]Benzothieno[3,2-b]pyran-2-one, 4-phenyl-, 5,5-dioxide (9CI) (CA INDEX NAME)



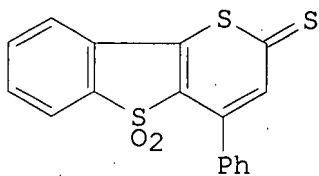
GI



I



II



III

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AB The title compound (I) was prepared in 45% yield by the cyclocondensation of benzothiophenone II with P4S10 in refluxing MeCN containing NaHCO3 for 1 h.

The isomeric compound III was prepared by the cyclocondensation of 2-HSC6H4CO2H with HO2CCH2CPh:CHCO2H followed by oxidation and disulfuration.

Several analogs of I and III were also prepared

L4 ANSWER 6 OF 16 CAPLUS COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER: 1983:53665 CAPLUS

DOCUMENT NUMBER: 98:53665

TITLE: Ring-expansion of some sulfur-containing heterocyclic

compounds with dimethyl acetylenedicarboxylate
AUTHOR(S): Lamm, Bo; Aurell, Carl Johan

CORPORATE SOURCE: Dep. Org. Chem., Chalmers Univ. Technol., Goeteborg,

S-412 96, Swed.

SOURCE: Acta Chemica Scandinavica, Series B: Organic Chemistry and Biochemistry (1982), B36(7), 435-42
CODEN: ACBOCV; ISSN: 0302-4369

DOCUMENT TYPE: Journal

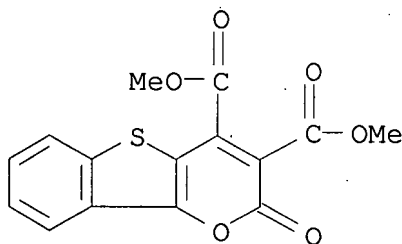
LANGUAGE: English

IT 84261-39-2P

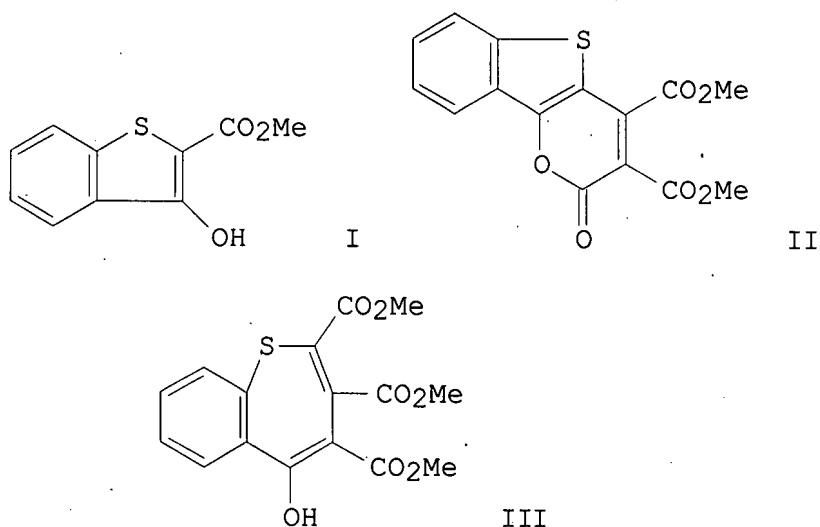
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)

RN 84261-39-2 CAPLUS

CN 2H-[1]Benzothieno[3,2-b]pyran-3,4-dicarboxylic acid, 2-oxo-, dimethyl ester (9CI) (CA INDEX NAME)



GI



AB Benzo[b]thiepin, benzo[b]thiocin, and benzo[b]thionin derivs. were prepared through [2+2] cycloaddn. of di-Me acetylenedicarboxylate to enamines, β -keto-ester anions and one β -diketone anion. In the addition to I a fluorescent by-product was identified as an α -pyrone-derivative (II) besides the main product III.

L4 ANSWER 7 OF 16 CAPLUS COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER: 1983:34484 CAPLUS

DOCUMENT NUMBER: 98:34484

TITLE: Thermolysis of
6-hydroxy-3,4,5-tris-methoxycarbonyl-2H-
benzo[b]thiocin

AUTHOR(S): Lamm, Bo; Aurell, Carl Johan

CORPORATE SOURCE: Dep. Org. Chem., Chalmers Univ. Technol.,
Goeteborg,

S-412 96, Swed.

SOURCE: Acta Chemica Scandinavica, Series B: Organic
Chemistry and Biochemistry (1982), B36(8), 566-8
CODEN: ACBOCV; ISSN: 0302-4369

DOCUMENT TYPE: Journal

LANGUAGE: English

OTHER SOURCE(S): CASREACT 98:34484

IT 84157-04-0P

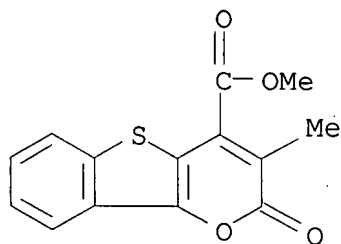
RL: FORM (Formation, nonpreparative); PREP (Preparation)
(formation of, from thermolysis of

hydroxybenzothiophenetricarboxylate)

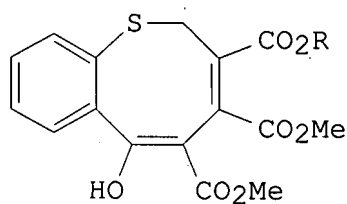
RN 84157-04-0 CAPLUS

CN 2H-[1]Benzothieno[3,2-b]pyran-4-carboxylic acid, 3-methyl-2-oxo-,
methyl

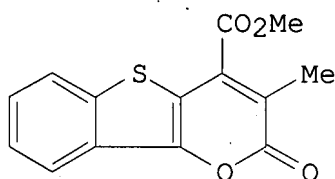
ester (9CI) (CA INDEX NAME)



GI



I



II

AB. Thermolysis of the title compound or its Et analog (I, R = Me, Et) gave the benzothienopyranone II. The structure of II was confirmed by independent synthesis from 3-hydroxybenzo[b]thiophene and MeO₂CCHMeCOCOMe.

L4 ANSWER 8 OF 16 CAPLUS COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER: 1978:44882 CAPLUS

DOCUMENT NUMBER: 88:44882

TITLE: Antitumor activity of heterocyclic and ketenethioacetal derivatives

AUTHOR(S): Kobayashi, Goro; Matsuda, Yoshiro; Tominaga, Yoshinori; Ohkuma, Mihoko; Shinoda, Hirotaka; Kohn,

Morihiro; Mizuno, Den'ichi
CORPORATE SOURCE: Fac. Pharm. Sci., Nagasaki Univ., Nagasaki, Japan
SOURCE: Yakugaku Zasshi (1977), 97(9), 1039-45

CODEN: YKKZAJ; ISSN: 0031-6903

DOCUMENT TYPE: Journal

LANGUAGE: Japanese

IT 57840-16-1P

RL: BAC (Biological activity or effector, except adverse); BSU (Biological

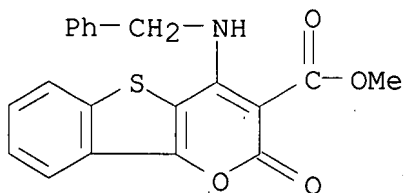
study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use);

BIOL (Biological study); PREP (Preparation); USES (Uses) (preparation and antitumor activity of)

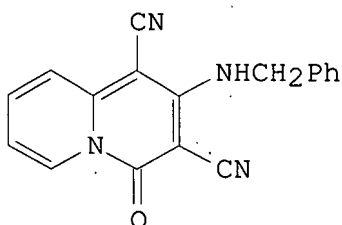
RN 57840-16-1 CAPLUS

10/552,459

CN 2H-[1]Benzothieno[3,2-b]pyran-3-carboxylic acid, 2-oxo-4-
[(phenylmethyl)amino]-, methyl ester (9CI) (CA INDEX NAME)



GI



I

AB Eighty-seven compds. of maleimide, five- or six-ring heterocyclic
4H-quinolizines, and ethylene derivs. were prepared and their antitumor
activity was examined using a solid type of Ehrlich carcinoma.
1,3-Dicyano-2-benzylamine-4H-quinolizin-4-one (I) [65125-90-8] had
some
antitumor effect, but no other synthesized compds. were effective.

L4 ANSWER 9 OF 16 CAPLUS, COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER: 1976:17052 CAPLUS

DOCUMENT NUMBER: 84:17052

TITLE: Heterocyclic ketenethioacetal derivatives. VI.
Synthesis and reaction of 2-

bis(methylthio)methylenebenzothiophen-3(2H)-one
AUTHOR(S): Tominaga, Yoshinori; Morita, Yuko; Matsuda,
Yoshiro;

Kobayashi, Goro
CORPORATE SOURCE: Fac. Pharm. Sci., Nagasaki Univ., Nagasaki, Japan
SOURCE: Chemical & Pharmaceutical Bulletin (1975), 23(10),
2390-6

CODEN: CPBTAL; ISSN: 0009-2363

DOCUMENT TYPE: Journal

LANGUAGE: English

OTHER SOURCE(S): CASREACT 84:17052

IT 57840-11-6P 57840-12-7P 57840-16-1P

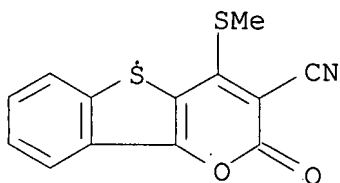
57840-17-2P

RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)

10/552,459

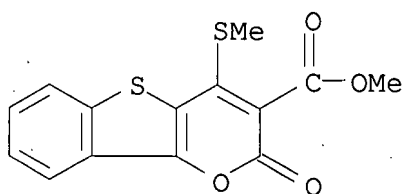
RN 57840-11-6 CAPLUS

CN 2H-[1]Benzothieno[3,2-b]pyran-3-carbonitrile, 4-(methylthio)-2-oxo-
(9CI)
(CA INDEX NAME)



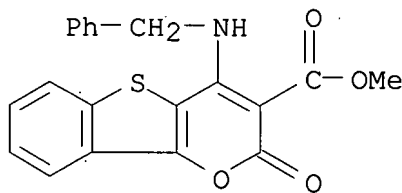
RN 57840-12-7 CAPLUS

CN 2H-[1]Benzothieno[3,2-b]pyran-3-carboxylic acid, 4-(methylthio)-2-oxo-,
methyl ester (9CI) (CA INDEX NAME)



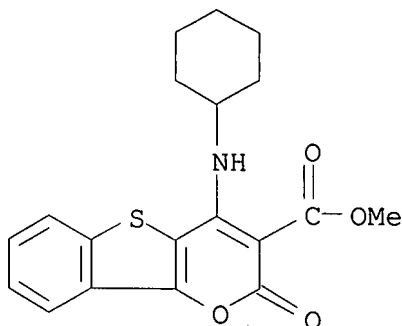
RN 57840-16-1 CAPLUS

CN 2H-[1]Benzothieno[3,2-b]pyran-3-carboxylic acid, 2-oxo-4-
[(phenylmethyl)amino]-, methyl ester (9CI) (CA INDEX NAME)



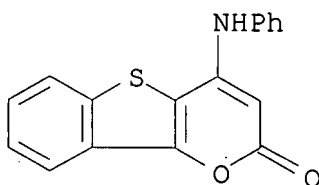
RN 57840-17-2 CAPLUS

CN 2H-[1]Benzothieno[3,2-b]pyran-3-carboxylic acid,
4-(cyclohexylamino)-2-oxo-
, methyl ester (9CI) (CA INDEX NAME)



AB 2-Bis(methylthio)methylenebenzothiophen-3(2H)-one, prepared by treatment of benzothiophen-3(2H)-one with CS, in Me2SO containing NaOH, reacted with nucleophilic reagents such as amines or active methylenes to give the corresponding replacement products of one or two methylthio groups in good yields.

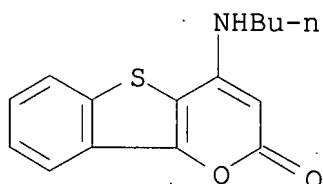
L4 ANSWER 10 OF 16 CAPLUS COPYRIGHT 2007 ACS on STN
 ACCESSION NUMBER: 1975:479110 CAPLUS
 DOCUMENT NUMBER: 83:79110
 TITLE: Action of amines on 4-hydroxy-2-oxo-2H-pyrano[3,2-b]thianaphthenes
 AUTHOR(S): Ali, Mohamed I.; Samy, Salah M.
 CORPORATE SOURCE: Fac. Sci., Cairo Univ., Giza, Egypt
 SOURCE: Egyptian Journal of Chemistry (1974), Volume Date 1973, (Spec. Issue), 169-77
 CODEN: EGJCA3; ISSN: 0449-2285
 DOCUMENT TYPE: Journal
 LANGUAGE: English
 IT 2035-56-5P 53324-54-2P 53324-55-3P
 53324-56-4P 53324-58-6P 53324-59-7P
 53324-60-0P
 RL: SPN (Synthetic preparation); PREP (Preparation)
 (preparation of)
 RN 2035-56-5 CAPLUS
 CN 2H-[1]Benzothieno[3,2-b]pyran-2-one, 4-(phenylamino)- (9CI) (CA INDEX NAME)



10/552,459

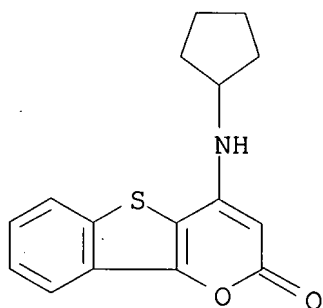
RN 53324-54-2 CAPLUS

CN 2H-[1]Benzothieno[3,2-b]pyran-2-one, 4-(butylamino)- (9CI) (CA INDEX NAME)



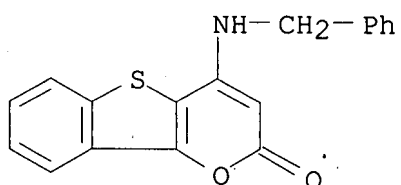
RN 53324-55-3 CAPLUS

CN 2H-[1]Benzothieno[3,2-b]pyran-2-one, 4-(cyclopentylamino)- (9CI) (CA INDEX NAME)



RN 53324-56-4 CAPLUS

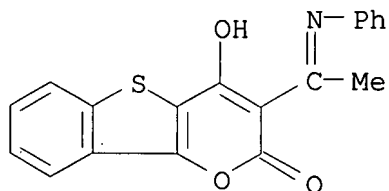
CN 2H-[1]Benzothieno[3,2-b]pyran-2-one, 4-[(phenylmethyl)amino]- (9CI)
(CA INDEX NAME)



RN 53324-58-6 CAPLUS

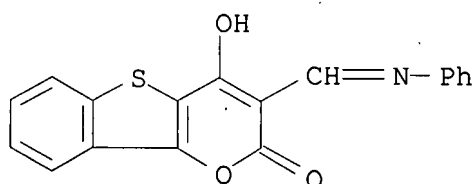
CN 2H-[1]Benzothieno[3,2-b]pyran-2-one,
4-hydroxy-3-[1-(phenylimino)ethyl]-
(9CI) (CA INDEX NAME)

10/552,459



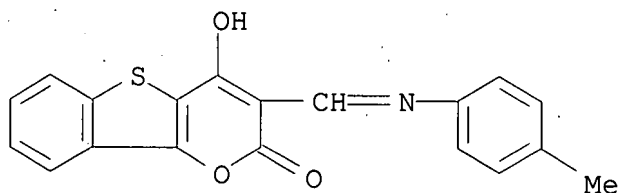
RN 53324-59-7 CAPLUS

CN 2H-[1]Benzothieno[3,2-b]pyran-2-one, 4-hydroxy-3-[(phenylimino)methyl]-
(9CI) (CA INDEX NAME)



RN 53324-60-0 CAPLUS

CN 2H-[1]Benzothieno[3,2-b]pyran-2-one, 4-hydroxy-3-[[4-methylphenyl]imino]methyl]- (9CI) (CA INDEX NAME)

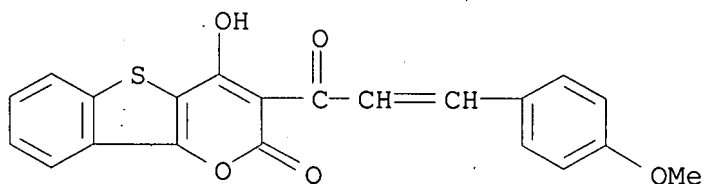


IT 2034-93-7 2035-18-9 6906-77-0
56342-51-9

RL: RCT (Reactant); RACT (Reactant or reagent)
(reaction with amines)

RN 2034-93-7 CAPLUS

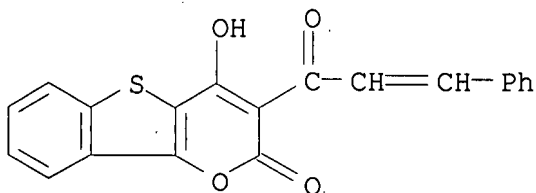
CN 2H-[1]Benzothieno[3,2-b]pyran-2-one,
4-hydroxy-3-[3-(4-methoxyphenyl)-1-oxo-2-propenyl]- (9CI) (CA INDEX NAME)



10/552,459

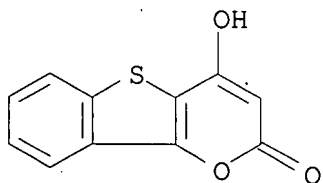
RN 2035-18-9 CAPLUS

CN 2H-[1]Benzothieno[3,2-b]pyran-2-one, 4-hydroxy-3-(1-oxo-3-phenyl-2-propenyl)- (9CI) (CA INDEX NAME)



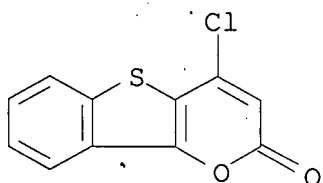
RN 6906-77-0 CAPLUS

CN 2H-[1]Benzothieno[3,2-b]pyran-2-one, 4-hydroxy- (9CI) (CA INDEX NAME)



RN 56342-51-9 CAPLUS

CN 2H-[1]Benzothieno[3,2-b]pyran-2-one, 4-chloro- (9CI) (CA INDEX NAME)



GI For diagram(s), see printed CA Issue.

AB 4-Hydroxypyrananthienaphthene (I, R = OH, R1 = H) (II) reacted with PhNH2

in boiling HOCHMe2 to give the ring-cleavage product (III, R2 = COCH2CONHPh) whereas at higher temperature (e.g., in refluxing phenetole) IV (R3

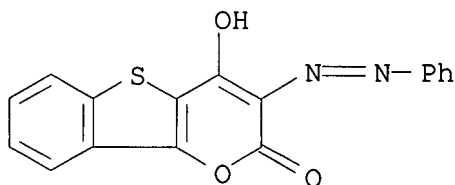
= Ph) was obtained; with H2NR4 (R4 = Bu, cyclopentyl, cyclohexyl, CH2CH2OH, CH2Ph) in boiling EtOH II gave only III [R2 = C(NHR4):CHCONHR4].

I (R = Cl, R1 = H) reacted with H2NR4 in EtOH to give the aminopyrananthienaphthenes (I, R = NHR4, R1 = H), and I (R = OH, R1 = COCH:CHR5, R5 = Ph, C6H4OMe-p) reacted with H2NPh to give V.

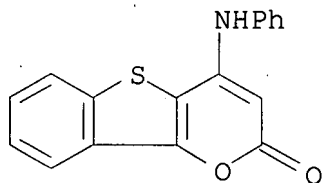
L4 ANSWER 11 OF 16 CAPLUS COPYRIGHT 2007 ACS on STN

10/552,459

ACCESSION NUMBER: 1974:449595 CAPLUS
DOCUMENT NUMBER: 81:49595
TITLE: Action of amines on 4-hydroxy-2-oxo-2H-pyrano[3,2-b]thianaphthenes
AUTHOR(S): Ali, Mohamed I.; Samy, Salah M.
CORPORATE SOURCE: Fac. Sci., Univ. Cairo, Giza, Egypt
SOURCE: Egyptian Journal of Chemistry (1973), (Special), 169-77
CODEN: EGJCA3; ISSN: 0449-2285
DOCUMENT TYPE: Journal
LANGUAGE: English
IT 2034-90-4P 2035-56-5P 53324-54-2P
53324-55-3P 53324-56-4P 53324-58-6P
53324-59-7P 53324-60-0P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)
RN 2034-90-4 CAPLUS
CN 2H-[1]Benzothieno[3,2-b]pyran-2-one, 4-hydroxy-3-(phenylazo)- (9CI)
(CA INDEX NAME)

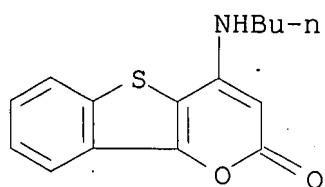


RN 2035-56-5 CAPLUS
CN 2H-[1]Benzothieno[3,2-b]pyran-2-one, 4-(phenylamino)- (9CI) (CA INDEX NAME)



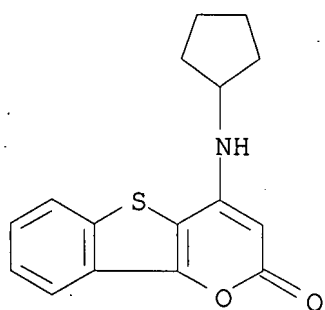
RN 53324-54-2 CAPLUS
CN 2H-[1]Benzothieno[3,2-b]pyran-2-one, 4-(butylamino)- (9CI) (CA INDEX NAME)

10/552,459



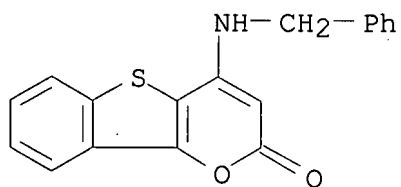
RN 53324-55-3 CAPLUS

CN 2H-[1]Benzothieno[3,2-b]pyran-2-one, 4-(cyclopentylamino)- (9CI) (CA INDEX NAME)



RN 53324-56-4 CAPLUS

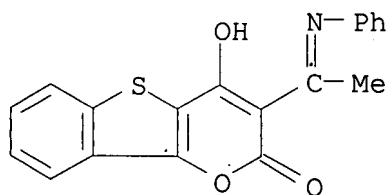
CN 2H-[1]Benzothieno[3,2-b]pyran-2-one, 4-[(phenylmethyl)amino]- (9CI) (CA INDEX NAME)



RN 53324-58-6 CAPLUS

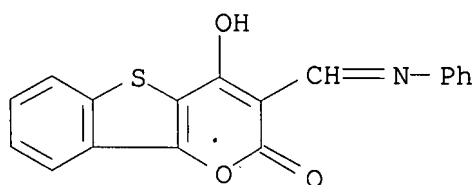
CN 2H-[1]Benzothieno[3,2-b]pyran-2-one, 4-hydroxy-3-[1-(phenylimino)ethyl]- (9CI) (CA INDEX NAME)

10/552,459



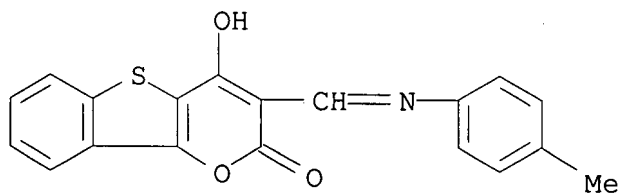
RN 53324-59-7 CAPLUS

CN 2H-[1]Benzothieno[3,2-b]pyran-2-one, 4-hydroxy-3-[(phenylimino)methyl]-
(9CI) (CA INDEX NAME)



RN 53324-60-0 CAPLUS

CN 2H-[1]Benzothieno[3,2-b]pyran-2-one, 4-hydroxy-3-[[4-methylphenyl]imino]methyl]- (9CI) (CA INDEX NAME)

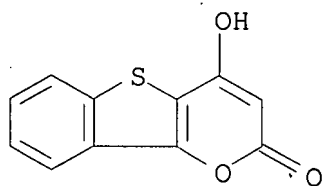


IT 6906-77-0

RL: RCT (Reactant); RACT (Reactant or reagent)
(reaction of, with amines)

RN 6906-77-0 CAPLUS

CN 2H-[1]Benzothieno[3,2-b]pyran-2-one, 4-hydroxy- (9CI) (CA INDEX NAME)



IT 2034-93-7 2035-18-9 2035-28-1

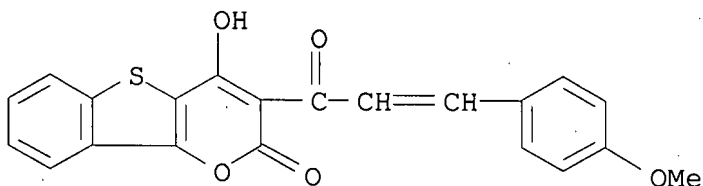
RL: RCT (Reactant); RACT (Reactant or reagent)

10/552,459

(reaction of, with aniline)

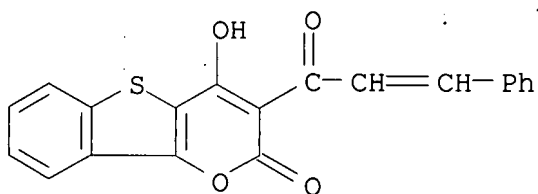
RN 2034-93-7 CAPLUS

CN 2H-[1]Benzothieno[3,2-b]pyran-2-one,
4-hydroxy-3-[3-(4-methoxyphenyl)-1-
oxo-2-propenyl]- (9CI) (CA INDEX NAME)



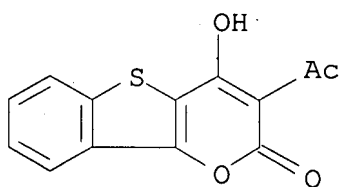
RN 2035-18-9 CAPLUS

CN 2H-[1]Benzothieno[3,2-b]pyran-2-one, 4-hydroxy-3-(1-oxo-3-phenyl-2-propenyl)- (9CI) (CA INDEX NAME)



RN 2035-28-1 CAPLUS

CN 2H-[1]Benzothieno[3,2-b]pyran-2-one, 3-acetyl-4-hydroxy- (9CI) (CA INDEX NAME)



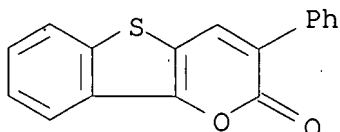
GI For diagram(s), see printed CA Issue.

AB The pyranothianaphthene I (R = OH, R1 = H) reacted with PhNH2 at .apprx.80-140° with ring-opening to give II (R2 = COCH2CONHPh), whereas at .apprx.170° I (R = NHPh, R1 = H) was obtained. Reaction in HOAc at 118° yielded I (R = NHPh, R1 = H), and II (R2 = Ac) in addition to PhNHAc Ring-opening also occurred in the reaction of I (R = OH, R1 = H) with R3NH2 (R3 = Bu, cyclopentyl, cyclohexyl, CH2CH2OH, CH2Ph) or morpholine to give II [R2 = C(:CHCONHR3)NHR3]. 3,3'-Methylenebis(4-

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hydroxy-2-oxo-2H-pyrano[3,2-b]thianaph-thene) also reacted with PhNH₂ at 180° to give I (R = NHPH, R₁ = H), but remained unchanged when the reaction was carried out in refluxing EtOH. I (R = OH, R₁ = COCH:CHPh, COCH:CHC₆H₄OMe-p) both reacted with PhNH₂ to give I (R = OH, R₁ = CMe:NPh). Reaction of I (R = OH, R₁ = H) with HC(:NC₆H₄R₄-p)NHC₆H₄R₄-p (R₄ = H, Me) gave I (R = OH, R₁ = CH:NC₆H₄R₄-p).

L4 ANSWER 12 OF 16 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 1967:115525 CAPLUS
DOCUMENT NUMBER: 66:115525
TITLE: Thiophene derivatives. XVI. The Vilsmeier-Haack reaction with 3- and 4-methoxybenzo[b]thiophene
AUTHOR(S): Ricci, Adolfo; Balucani, Dante; Buu-Hoi, N. P.
CORPORATE SOURCE: Univ. Studi, Perugia, Italy
SOURCE: Journal of the Chemical Society [Section] C: Organic
(1967), (8), 779-80
CODEN: JSOOAX; ISSN: 0022-4952
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 66:115525
IT 14854-19-4P, 2H-[1]Benzothieno[3,2-b]pyran-2-one, 3-phenyl-
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)
RN 14854-19-4 CAPLUS
CN 2H-[1]Benzothieno[3,2-b]pyran-2-one, 3-phenyl- (8CI) (CA INDEX NAME)

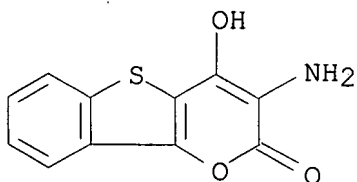


GI For diagram(s), see printed CA Issue.
AB The Vilsmeier-Haack formylation of 3-methoxybenzo[b]thiophene (I) at moderate temperature leads to 2-formyl-3-methoxybenzo[b]thiophene, and under more drastic conditions, to 3-chloro-2-formylbenzo[b]thiophene. 4-Methoxybenzo[b]thiophene undergoes formylation in the benzene ring, to give 7-formyl-4-methoxybenzo[b]thiophene.

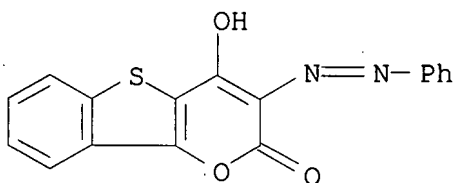
L4 ANSWER 13 OF 16 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 1966:447553 CAPLUS
DOCUMENT NUMBER: 65:47553
ORIGINAL REFERENCE NO.: 65:8852e-h
TITLE: Syntheses of heterocycles. LXXXI. Substituted glyoxal hydrazones
AUTHOR(S): Ziegler, E; Eichenseer, F

10/552,459

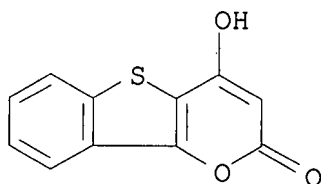
CORPORATE SOURCE: Univ. Graz, Austria
SOURCE: Monatshefte fuer Chemie (1966), 97(2), 391-7
CODEN: MOCMB7; ISSN: 0026-9247
DOCUMENT TYPE: Journal
LANGUAGE: German
OTHER SOURCE(S): CASREACT 65:47553
IT 6906-80-5
(Derived from data in the 7th Collective Formula Index (1962-1966))
RN 6906-80-5 CAPLUS
CN Benzo[b]thiophene-2-acrylic acid, α -amino- β ,3-dihydroxy-,
 δ -lactone (7CI, 8CI) (CA INDEX NAME)



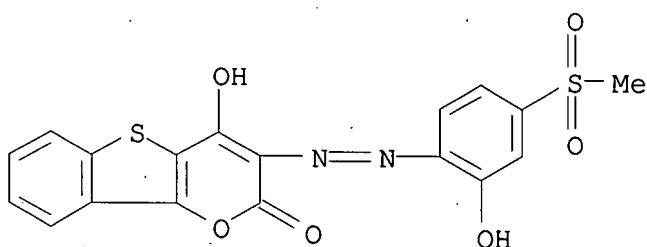
IT 2034-90-4P, Benzo[b]thiophene-2-acrylic acid, β ,3-dihydroxy-
 α -(phenylazo)-, δ -lactone 6906-77-0P,
Benzo[b]thiophene-2-acrylic acid, β ,3-dihydroxy-, δ -lactone
6906-86-1P, Benzo[b]thiophene-2-acrylic acid, β ,3-dihydroxy-
 α -[[2-hydroxy-4-(methylsulfonyl)phenyl]azo]-, δ -lactone
RL: PREP (Preparation)
(preparation of)
RN 2034-90-4 CAPLUS
CN 2H-[1]Benzothieno[3,2-b]pyran-2-one, 4-hydroxy-3-(phenylazo)- (9CI)
(CA INDEX NAME)



RN 6906-77-0 CAPLUS
CN 2H-[1]Benzothieno[3,2-b]pyran-2-one, 4-hydroxy- (9CI) (CA INDEX NAME)



RN 6906-86-1 CAPLUS

CN Benzo[b]thiophene-2-acrylic acid, β ,3-dihydroxy- α -[[2-hydroxy-4-(methylsulfonyl)phenyl]azo]-, δ -lactone (7CI, 8CI) (CA INDEX NAME)

AB cf. CA 65, 7137f. The syntheses were started with the known 4-hydroxy-2-oxoin-deno[1,2-b]pyran (I), its O analogs (II), m. 212°, and its S analog (III), m. 257-9°, both of which were prepared by heating the 3benzyl derivative at 140° 10 min. with AlCl₃ and

acidifying with HCl. I, II, and III were then coupled with diazotized aniline or 5-methylsulfonyl-2-aminophenol in about 10% Na₂CO₃ to give IV,

m. 241°, V, m. 264°, VI, m. 253-5°, VII, m. 350°, VIII, m. 285°, and IX, m. 250°, in more than 80% yields. These upon hydrolysis with boiling 3% KOH in dilute EtOH 1-3

hrs. gave XI, m 188-90°, XII, m. 198-200°, XIII, m. 222° (diacetate m. 162°), XIV, m. 224-6°, and XV, m. 223°, in more than 75% yields. In the case of IV the intermediate carboxylic acid (X), m. 163°, was isolated in 75% yield by limiting the time of hydrolysis to 5 min. XI gave with CH₂N₂ a diacetate (XVa), m.

180°, and upon boiling with NH₂OH in EtOH 48 hrs., the trioxime (XVI), m. 205-7°. With PhNHNH₂·HCl and NaOAc it gave a pyrazolone (XVII), m. 223°. The N-methyl derivative, m. 205°, could be obtained either from XVa by the action of PhNHNH₂ or from XVII with CH₂N₂.

L4 ANSWER 14 OF 16 CAPLUS COPYRIGHT 2007 ACS on STN

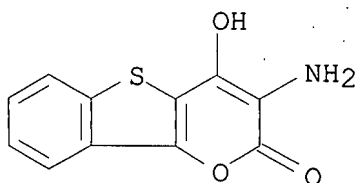
ACCESSION NUMBER: 1966:447552 CAPLUS

DOCUMENT NUMBER: 65:47552

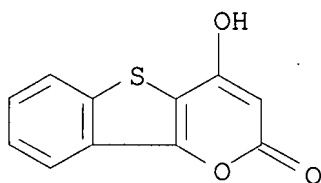
ORIGINAL REFERENCE NO.: 65:8852d-e

10/552,459

TITLE: Removal of thiophene from benzene by freezing out
AUTHOR(S): Smol'yaninova, N. M.; Smol'yaninova, S. I.;
Potarskii, V. K.
SOURCE: Izvestiya Tomskogo Politekhnikheskogo Instituta
(1965), 136, 93-6
From: Ref. Zh., Khim. 1966(5), Pt. II, Abstr. No.
5N116.
CODEN: ITPKAM; ISSN: 0368-0487
DOCUMENT TYPE: Journal
LANGUAGE: Russian
IT 6906-80-5
(Derived from data in the 7th Collective Formula Index (1962-1966))
RN 6906-80-5 CAPLUS
CN Benzo[b]thiophene-2-acrylic acid, α -amino- β ,3-dihydroxy-,
 δ -lactone (7CI, 8CI) (CA INDEX NAME)



IT 6906-77-0P, Benzo[b]thiophene-2-acrylic acid, β ,3-dihydroxy-,
 δ -lactone
RL: PREP (Preparation)
(preparation of)
RN 6906-77-0 CAPLUS
CN 2H-[1]Benzo[hieno[3,2-b]pyran-2-one, 4-hydroxy- (9CI) (CA INDEX NAME)



AB The dependence of C₆H₆ yield, its thiophene content, and the degree of purification on the number of crystallization steps from a mixture of xylenes or MeOH was studied. Thiophene can be removed from C₆H₆ by a freezingout method with MeOH as solvent. A high-purity product can be obtained by multiple purifications with a high recirculation factor.

L4 ANSWER 15 OF 16 CAPLUS COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER: 1965:90854 CAPLUS
 DOCUMENT NUMBER: 62:90854
 ORIGINAL REFERENCE NO.: 62:16218g-h,16219a-h,16220a-c
 TITLE: Synthesis of substituted linear furano[2,3-g][1]benzopyrones and [3,2-b]thianaphthenopyrones
 AUTHOR(S): Mustafa, A.; Asker, W.; Hishmat, O. H.; Ali, M. I.; Mansour, A. K. E.; Abed, N. M.; Khalil, K. M. A.; Samy, S. M.
 CORPORATE SOURCE: Cairo Univ.
 SOURCE: Tetrahedron (1965), 21(4), 849-59
 CODEN: TETRAB; ISSN: 0040-4020
 DOCUMENT TYPE: Journal
 LANGUAGE: English
 OTHER SOURCE(S): CASREACT 62:90854
 IT 2034-88-0P, Benzo[b]thiophene-2-acrylic acid, β ,3-dihydroxy- α -(p-tolylazo)-, δ -lactone 2034-89-1P, Benzo[b]thiophene-2-acrylic acid, α -[(p-chlorophenyl)azo]- β ,3-dihydroxy-, δ -lactone 2034-90-4P, Benzo[b]thiophene-2-acrylic acid, β ,3-dihydroxy- α -(phenylazo)-, δ -lactone 2034-91-5P, Benzo[b]thiophene-2-acrylic acid, α -acetamido- β ,3-dihydroxy-, δ -lactone 2034-92-6P, Benzo[b]thiophene-2-acrylic acid, β ,3-dihydroxy- α -nitro-, δ -lactone 2034-93-7P, Benzo[b]thiophene-2-acrylic acid, β ,3-dihydroxy- α -(p-methoxycinnamoyl)-, δ -lactone 2035-18-9P, Benzo[b]thiophene-2-acrylic acid, α -cinnamoyl- β ,3-dihydroxy-, δ -lactone 2035-19-0P, Benzo[b]thiophene-2-acrylic acid, α -acetyl- β ,3-dihydroxy-, δ -lactone, methylphenylhydrazone 2035-20-3P, Benzo[b]thiophene-2-acrylic acid, β ,3-dihydroxy- α -(N-phenylbutyrimidoyl)-, δ -lactone 2035-21-4P, Benzo[b]thiophene-2-acrylic acid, β ,3-dihydroxy- α -(N-phenylpropionimidoyl)-, δ -lactone 2035-22-5P, Benzo[b]thiophene-2-acrylic acid, β ,3-dihydroxy- α -(N-p-tolylacetimidoyl)-, δ -lactone 2035-23-6P, Benzo[b]thiophene-2-acrylic acid, α -(N-butylacetimidoyl)- β ,3-dihydroxy-, δ -lactone 2035-24-7P, Benzo[b]thiophene-2-acrylic acid, α -(N-ethylacetimidoyl)- β ,3-dihydroxy-, δ -lactone 2035-25-8P, Benzo[b]thiophene-2-acrylic acid, α -acetimidoyl- β ,3-dihydroxy-, δ -lactone 2035-26-9P, Benzo[b]thiophene-2-acrylic acid, α -butyryl- β ,3-dihydroxy-, δ -lactone 2035-27-0P, Benzo[b]thiophene-2-acrylic acid, β ,3-dihydroxy- α -propionyl-, δ -lactone 2035-28-1P, Benzo[b]thiophene-2-acrylic acid, α -acetyl- β ,3-dihydroxy-, δ -lactone 2035-29-2P, Benzo[b]thiophene-2-acrylic acid, β ,3-dihydroxy-, δ -lactone, benzoate 2035-30-5P, Benzo[b]thiophene-2-acrylic acid, 3-hydroxy- β -p-toluidino-, δ -lactone 2035-56-5P, Benzo[b]thiophene-2-acrylic acid, β -anilino-3-hydroxy-, δ -lactone 2239-09-0P, Benzo[b]thiophene-2-acrylic acid, α -(N-sec-butylacetimidoyl)- β ,3-dihydroxy-, δ -lactone 2239-10-3P, Benzo[b]thiophene-2-acrylic acid, β ,3-dihydroxy- α -(phenylacetyl)-, δ -lactone 2239-11-4P,

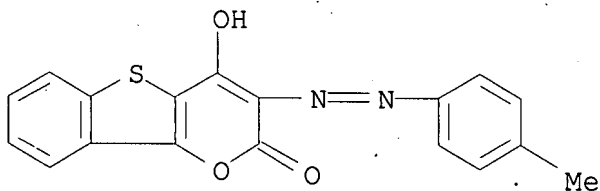
10/552,459

Benzo[b]thiophene-2-acrylic acid, β ,3-dihydroxy- α -isobutyryl-,
 δ -lactone 2864-01-9P, Benzo[b]thiophene-2-acrylic acid,
 β ,3-dihydroxy- α -(N-isobutylacetimidoyl)-, δ -lactone
RL: PREP (Preparation)

(preparation of)

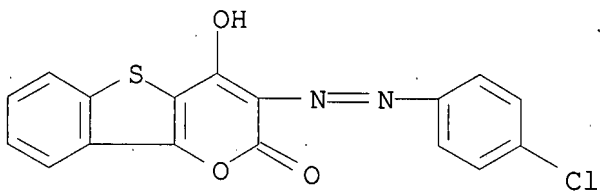
RN 2034-88-0 CAPLUS

CN Benzo[b]thiophene-2-acrylic acid, β ,3-dihydroxy- α -(p-tolylazo)-
, δ -lactone (7CI, 8CI) (CA INDEX NAME)



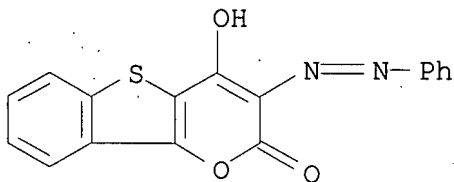
RN 2034-89-1 CAPLUS

CN 2H-[1]Benzothieno[3,2-b]pyran-2-one, 3-[(4-chlorophenyl)azo]-4-hydroxy-
(9CI) (CA INDEX NAME)



RN 2034-90-4 CAPLUS

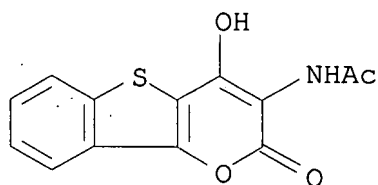
CN 2H-[1]Benzothieno[3,2-b]pyran-2-one, 4-hydroxy-3-(phenylazo)- (9CI)
(CA INDEX NAME)



RN 2034-91-5 CAPLUS

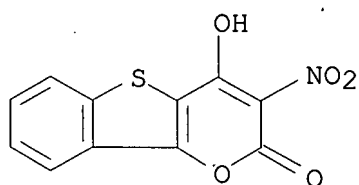
CN Benzo[b]thiophene-2-acrylic acid, α -acetamido- β ,3-dihydroxy-,
 δ -lactone (7CI, 8CI) (CA INDEX NAME)

10/552,459



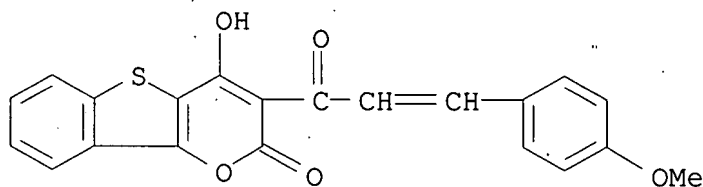
RN 2034-92-6 CAPLUS

CN Benzo[b]thiophene-2-acrylic acid, β ,3-dihydroxy- α -nitro-,
 δ -lactone (7CI, 8CI) (CA INDEX NAME)



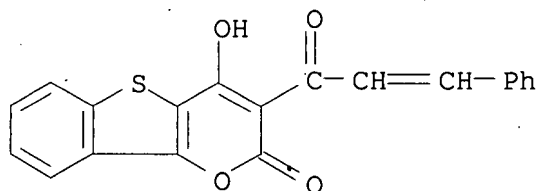
RN 2034-93-7 CAPLUS

CN 2H-[1]Benzothieno[3,2-b]pyran-2-one,
4-hydroxy-3-[3-(4-methoxyphenyl)-1-
oxo-2-propenyl]- (9CI) (CA INDEX NAME)



RN 2035-18-9 CAPLUS

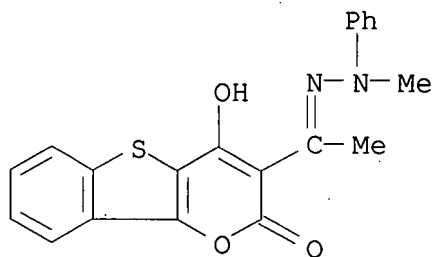
CN 2H-[1]Benzothieno[3,2-b]pyran-2-one, 4-hydroxy-3-(1-oxo-3-phenyl-2-
propenyl)- (9CI) (CA INDEX NAME)



RN 2035-19-0 CAPLUS

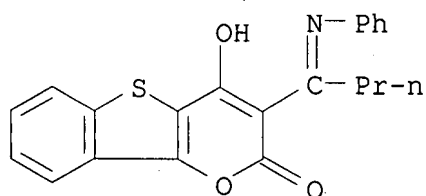
CN 2H-[1]Benzothieno[3,2-b]pyran-2-one, 4-hydroxy-3-[1-
(methylphenylhydrazono)ethyl]- (9CI) (CA INDEX NAME)

10/552,459



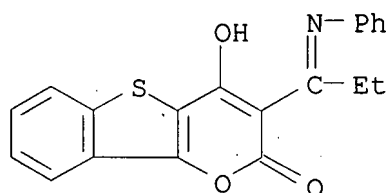
RN 2035-20-3 CAPLUS

CN Benzo[b]thiophene-2-acrylic acid, β ,3-dihydroxy- α -(N-phenylbutyrimidoyl)-, δ -lactone (7CI, 8CI) (CA INDEX NAME)



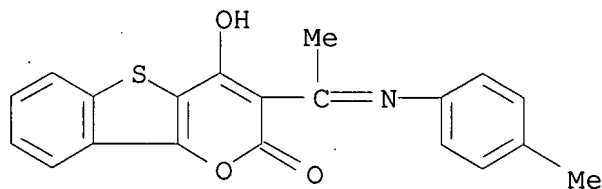
RN 2035-21-4 CAPLUS

CN Benzo[b]thiophene-2-acrylic acid, β ,3-dihydroxy- α -(N-phenylpropionimidoyl)-, δ -lactone (7CI, 8CI) (CA INDEX NAME)



RN 2035-22-5 CAPLUS

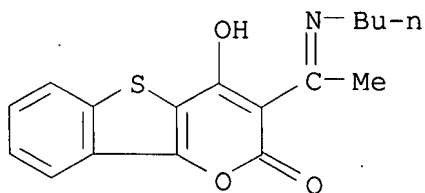
CN Benzo[b]thiophene-2-acrylic acid, β ,3-dihydroxy- α -(N-p-tolylacetimidoyl)-, δ -lactone (7CI, 8CI) (CA INDEX NAME)



RN 2035-23-6 CAPLUS

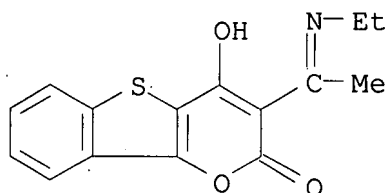
10/552,459

CN 2H-[1]Benzothieno[3,2-b]pyran-2-one, 3-[1-(butylimino)ethyl]-4-hydroxy-
(9CI) (CA INDEX NAME)



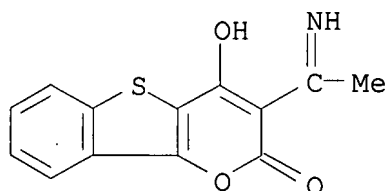
RN 2035-24-7 CAPLUS

CN Benzo[b]thiophene-2-acrylic acid, α -(N-ethylacetimidoyl)- β ,3-dihydroxy-, δ -lactone (7CI, 8CI) (CA INDEX NAME)



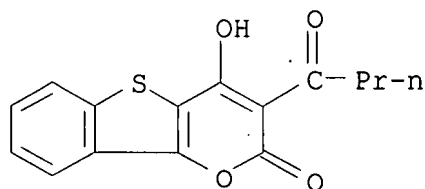
RN 2035-25-8 CAPLUS

CN Benzo[b]thiophene-2-acrylic acid, α -acetimidoyl- β ,3-dihydroxy-, δ -lactone (7CI, 8CI) (CA INDEX NAME)



RN 2035-26-9 CAPLUS

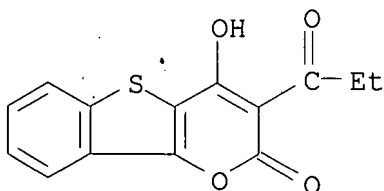
CN 2H-[1]Benzothieno[3,2-b]pyran-2-one, 4-hydroxy-3-(1-oxobutyl)- (9CI)
(CA INDEX NAME)



10/552,459

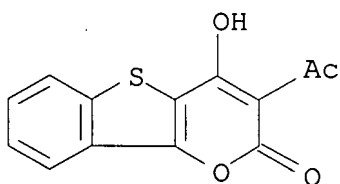
RN 2035-27-0 CAPLUS

CN Benzo[b]thiophene-2-acrylic acid, β ,3-dihydroxy- α -propionyl-,
 δ -lactone (7CI, 8CI) (CA INDEX NAME)



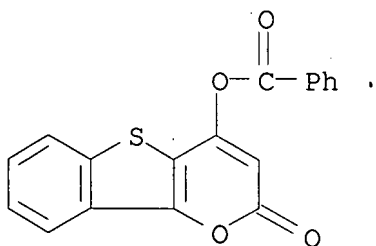
RN 2035-28-1 CAPLUS

CN 2H-[1]Benzothieno[3,2-b]pyran-2-one, 3-acetyl-4-hydroxy- (9CI) (CA
INDEX NAME)



RN 2035-29-2 CAPLUS

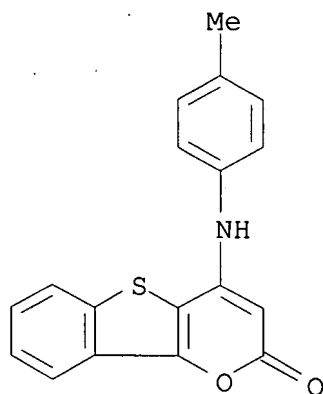
CN Benzo[b]thiophene-2-acrylic acid, β ,3-dihydroxy-, δ -lactone,
benzoate (7CI, 8CI) (CA INDEX NAME)



RN 2035-30-5 CAPLUS

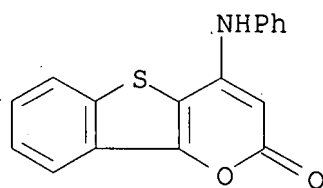
CN Benzo[b]thiophene-2-acrylic acid, 3-hydroxy- β -p-toluidino-,
 δ -lactone (7CI, 8CI) (CA INDEX NAME)

10/552,459



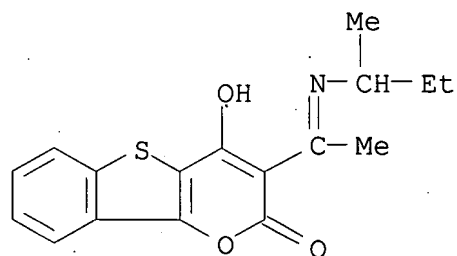
RN 2035-56-5 CAPLUS

CN 2H-[1]Benzo[thieno[3,2-b]pyran-2-one, 4-(phenylamino)- (9CI) (CA INDEX NAME)



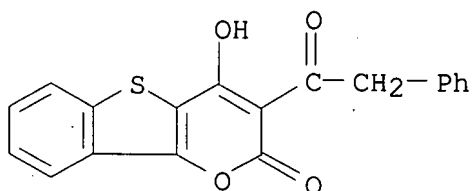
RN 2239-09-0 CAPLUS

CN Benzo[b]thiophene-2-acrylic acid, α -(N-sec-butylacetimidoyl)- β ,3-dihydroxy-, δ -lactone (7CI, 8CI) (CA INDEX NAME)

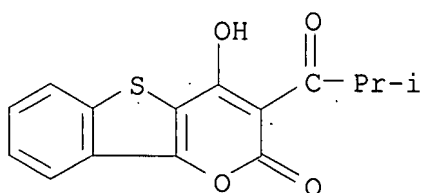


RN 2239-10-3 CAPLUS

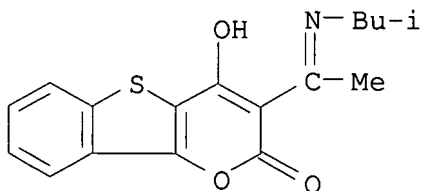
CN Benzo[b]thiophene-2-acrylic acid, β ,3-dihydroxy- α -(phenylacetyl)-, δ -lactone (8CI) (CA INDEX NAME)



RN 2239-11-4 CAPLUS

CN Benzo[b]thiophene-2-acrylic acid, β ,3-dihydroxy- α -isobutyryl-,
 δ -lactone (7CI, 8CI) (CA INDEX NAME)

RN 2864-01-9 CAPLUS

CN 2H-[1]Benzo[thieno[3,2-b]pyran-2-one, 4-hydroxy-3-[1-[(2-
methylpropyl)imino]ethyl]- (9CI) (CA INDEX NAME)

GI For diagram(s), see printed CA Issue.

AB Dry PhNO₂ (10 ml.) and 0.6 g. acetoxy-2,3-diphenylbenzofuran (I, R =
Ac,

R1 = H) kept 5 days at 25° with 1 g. anhydrous AlCl₃ and the dried
product extracted with ligroine (b. 100-40°) gave 73% I (R = H, R1 =
Ac) (II), m. 157° (alc.). I (R = R1 = H) (III) (2.8 g.) and 3.5 g.
AlCl₃ in 25 ml. PhNO₂ kept 5 days at 25° with 8 ml. AcCl, extracted
with ligroine and the crystalline product recrystd. from C₆H₆ yielded

12%

4-acetyl-5-hydroxy-2,3-diphenylbenzofuran, m. 291°. Concentration of
the

ligroine mother liquor gave 65% II. III (2.8 g.), and 1.86 g.

PhCH:CHCOCl

refluxed 3 hrs. with 3.4 g. AlCl₃ in 25 ml. CS₂ and the product
extracted with

petr. ether (b. 40-60°) yielded 95% I (R = PhCH:CHCO, R1 = H), m.
132° (alc.), converted by keeping in PhNO₂ with AlCl₃ to I (R = H,

$R_1 = \text{PhCH:CHCO}$), m. 184° , giving a reddish brown color with aqueous FeCl_3 . Treatment of III with PhCH:CHCOCl under Friedel-Crafts conditions gave 85% yield. II (1 g.) in 20 ml. EtOAc refluxed 1 hr. with 1 g. finally divided Na and the mixture decomposed with ice- H_2O , washed with Et 2O and the aqueous layer acidified with dilute HCl yielded 82% I ($R = \text{H}$, $R_1 = \text{AcCH}_2\text{CO}$) (IV). II (1 g.) and 4 ml. Et 2CO_3 shaken 5 min. with 0.5 g. Na at 25° and the mixture kept at 100° 4 hrs., the product taken up in H_2O and the solution washed with Et 2O , the aqueous layer acidified with cold dilute HCl gave 0.7 g. 2,3-diphenyl-8-hydroxy-6H-furano[2,3-g][1]benzopyran-6-one (V), m. $288-90^\circ$ (decomposition), N.M.R. singlets at 7.92, 7.18 ppm. and a signal group at 7.4 ppm. IV (1 g.) refluxed 1 hr. in 30 ml. 25% aqueous H_2SO_4 and the solution neutralized with Na_2CO_3 yielded 77% 2,3-diphenyl-6-methyl-8H-furano[2,3-g][1]benzopyran-8-one (VI), m. $211-12^\circ$, N.M.R. signals at 8.24, 7.4, 6.14, 2.35 ppm. The substitution of the 2- and 3-Ph groups effected the stabilization of V and VI against the action of mineral acids. III refluxed with $\text{H}_2\text{C:CHCH}_2\text{Br}$ and K_2CO_3 in dry Me_2CO 12 hrs. yielded 55% I ($R = \text{CH}_2\text{:CHCH}_2$, $R_1 = \text{H}$), m. 72° , rearranged by refluxing 3 hrs. in PhNMe_2 and acidifying the product to give I ($R = \text{H}$, $R_1 = \text{CH}_2\text{:CHCH}_2$), m. 83° , giving a red color with concentrated H_2SO_4 . The thianaphthene (VII, $R = \text{H}$, $R_1 = \text{OH}$) (VIII) (1 g.) (Smiles and Hart, CA 18, 390) heated with 1 ml. PhNH_2 in 20 ml. alc. or in the absence of alc. 4 hrs. on a water bath yielded 85% α -(3-hydroxy-2-thianaphthenoyl)acetanilide (IX, $R = \text{Ph}$) (X), m. $188-90^\circ$ (alc.). Similarly VIII and p-MeC $_6$ H $_4$ NH $_2$ heated in alc. gave 60% IX ($R = \text{p-MeC}_6\text{H}_4$), m. 199° (alc.). X (0.6 g.) and 1 ml. PhNH_2 heated 1.5 hrs. at 180° and the product triturated with cold alc. gave VII ($R = \text{H}$, $R_1 = \text{NHPh}$) (XI), m. 280° . Concentration of the mother liquor gave a compound tentatively formulated as IX [$R = \text{C(NHPh):CHCONHPh}$], m. 222° , giving a green color with aqueous FeCl_3 . VIII heated 1.5 hrs. with p-MeC $_6$ H $_4$ NH $_2$ gave 71% VII ($R = \text{H}$, $R_1 = \text{p-MeC}_6\text{H}_4\text{NH}$), m. $269-70^\circ$ (alc.). VIII benzoylated and crystallized from alc. yielded 75% VII ($R = \text{H}$, $R_1 = \text{OBz}$), m. 162° , converted by refluxing with PhNH_2 in alc. to X. VII ($R = \text{H}$, $R_1 = \text{Cl}$) refluxed in alc. with PhNH_2 yielded XI. VIII (0.01 mole), 8 ml. RCO $_2\text{H}$, and 10 ml. POCl $_3$ refluxed 45 min. and the mixture poured onto ice, the precipitate washed with cold H_2O and dried gave the acyl derivs. VII [R , R_1 , m.p. (solvent), and % yield given]: Ac, OH (XII), $189-90^\circ$ (AcOH), 76; EtCO, OH (XIII), $180-1^\circ$ (AcOH), 65; PrCO, OH (XIV), $170-1^\circ$ (AcOH), 76; Me $_2$ CHCO, OH, $172-3^\circ$

(AcOH), 70; PhCH₂CO, OH, 205° (dioxane), 71. The acyl derivs. XII-XIV (0.5 g.) refluxed 3-4 hrs. with excess of the appropriate amine (8 hrs. with NH₄OAc) in 30 ml. alc. gave the corresponding amino or imino derivs. (XV) as listed [R, R₁, m.p. (solvent), and % yield given]: Me, H, 288-90° (xylene), 80; Me, Et, 224° (alc.), 73; Me, Bu, 128-9° (aqueous alc.), 90; Me, EtMeCH, 139-40° (aqueous alc.), 83; Me, Me₂CHCH₂, 109-10° (aqueous alc.), 90; Me, p-MeC₆H₄, 228-30° (AcOH) 82; Et, Ph, 200° (alc.), 80; Pr, Ph, 145° (alc.), 72. XII and MePhNNH₂ refluxed in alc. 3 hrs. and the product recrystd. yielded 82% XV (R = Me, R₁ = NMePh), m. 168°. XII heated with BzH in the presence of a drop of piperidine 1 hr. on a water bath yielded 65% VII (R = COCH:CHR₂, R₁ = OH) (XVI, R₂ = Ph), m. 230° (dioxane-H₂O). Similarly was obtained 60% XVI (R₂ = p-MeOC₆H₄), m. 220° (dioxane). The ir spectrum of XII showed a broad OH absorption band as well as a strong peak in good agreement with the spectra of α,β -unsatd. δ -lactones. VIII gave bands at 7.55 and 5.87 μ but displayed no free OH peak, indicating a strongly H-bonded OH group. VIII kept 16 hrs. at 25° in AcOH with concentrated HNO₃ gave VII (R = NO₂, R₁ = OH), m. 215° (AcOH), reduced with Zn dust in 1:1 AcOH-Ac₂O to give VII (R = NHAc, R₁ = OH), m. 250-2°. VIII (1 g.) in 100 ml. alc. containing 2.5 g. NaOAc.3H₂O treated with 0.005 mole of the appropriate aryl diazonium chloride gave 94% VII (R = PhN:N, R₁ = OH), m. 260°, converted by reductive acetylation to yield 70% VII (R = NHAc, R₁ = OH), m. 250-2°; 84% VII (R = p-MeC₆H₄N:N, R₁ = OH), m. 250° (AcOH); and 85% VII (R = p-ClC₆H₄N:N, R₁ = OH), m. 257° (AcOH). EtOH (10 ml.) containing 0.001 mole 2-acetyl-3-hydroxythianaphthene, treated with 0.0015 mole of the appropriate aldehyde, RCHO, and the mixture refluxed 30 min. with 4 ml. 10% alc. NaOH, kept at 25°, and acidified with dilute HCl, filtered and the dried products crystallized from AcOH gave the 2-cinnamoyl-3-hydroxythianaphthenes (XVII) (R, m.p., and % yield): Ph, 154°, 50; p-MeOC₆H₄ (XVIII), 175°, 60; p-MeC₆H₄ (XIX), 130°, 65; 3,4-(OCH₂O)C₆H₃ (XX), 199°, 75; 3,4-(EtO)₂C₆H₃ (XXI), 150°, 50; p-ClC₆H₄ (XXII), 166°, 70. Each of the chalcones XX-XXII (0.5 g.) refluxed 10-15 hrs. with 0.5 g. SeO₂ in 8 ml. isoamyl alc. and the filtered solution evaporated, the residue washed with cold alc. and crystallized from alc. gave the 2-aryl-4-oxo-4H-pyrano[3,2-b]thianaphthenes (XXIII) (R, m.p., and % yield given): 3,4-(OCH₂O)C₆H₃, 266-7°, 80; 3,4-(EtO)₂C₆H₃, 170-1°, 65; p-ClC₆H₄, 235°, 80. Each of the chalcones XVIII-XXI (0.5 g.) and 0.5 g. of the appropriate thiol heated 4 hrs. on a water bath with 1-2 drops of piperidine, the product triturated with petr. ether and the solid crystallized gave the thiol adducts (XXIV) [R, R₁, m.p. (solvent) and % yield given]:

p-MeOC₆H₄, p-MeC₆H₄ (XXV), 101-2° (alc.), 60; p-MeC₆H₄, Ph (XXVI), 110-12° (AcOH), 55; p-MeC₆H₄, m-MeC₆H₄, 92-3° (alc.), 60; p-MeC₆H₄, p-MeC₆H₄, 105-6° (alc.), 60; 3,4-(OC-H₂O)C₆H₃, Ph, 125-6° (AcOH), 58; 3,4-(OCH₂O)C₆H₃, o-MeC₆H₄, 132-3° (AcOH), 60; 3,4-(OCH₂O)C₆H₃, m-MeC₆H₄, 106° (AcOH), 60; 3,4-(OCH₂O)C₆H₃, p-MeC₆H₄, 135-6° (AcOH), 60; 3,4-(EtO)₂C₆H₃, p-MeC₆H₄, 105° (alc.), 50. XXVI (0.5 g.) in 10 ml. alc. refluxed 30 min. with 3 ml.

5%

alc. KOH and the product taken up in 10 ml. cold alc., acidified with cold

dilute HCl and the product crystallized from AcOH gave XIX. Treatment of XVIII

or XX in AcOH with 30% H₂O₂ gave the dioxides [XXVII, R = p-MeOC₆H₄, 3,4-(OCH₂O)C₆H₃] (XXVIII, XXIX), m. 215° (AcOH), 271-3°

(PhCl), in 61 and 70% yields, resp. XXIX was also obtained in 52%

yield

by treatment of the thiol adduct XXIV [R = 3,4-(OCH₂O)C₆H₃, R₁ = p-MeC₆H₄]

with H₂O₂ in AcOH. XXVIII and XXIX formed unstable thiol adducts with p-thiocresol.

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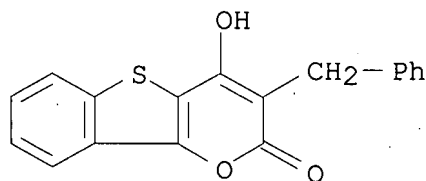
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IT 108237-18-9P, Benzo[b]thiophene-2-acrylic acid, α-benzyl-β,3-dihydroxy-, δ-lactone

RL: PREP (Preparation)
(preparation of)

RN 108237-18-9 CAPLUS

CN Benzo[b]thiophene-2-acrylic acid, α-benzyl-β,3-dihydroxy-, δ-lactone (6CI) (CA INDEX NAME)



GI For diagram(s), see printed CA Issue.

AB cf. CA 53, 20044g. The reactions of a number of cyclic ketones with $\text{PhCH}_2\text{CH}(\text{CO}_2\text{C}_6\text{H}_3\text{Cl}_2-2,4)_2$ (I) were reported. 1-Menthone (2 g.) and 4.84 g.

I heated 90 min. at 270° , the crude product steam distilled, the residual material dissolved in NaOH and repptd. with HCl, the material (2.8 g.) rubbed with 4:1 cyclohexane- C_6H_6 , allowed to stand several days,

and recrystd. from C_6H_6 or EtOAc gave 3-benzyl-4-hydroxy-5-methyl-8-isopropyl-5,6,7,8-tetrahydrocoumarin, m. 170° .

1-Phenyl-3-methyl-5-pyrazolone (3.5 g.) and 4.8 g. I heated 20 min. at 190° and the product rubbed with C_6H_6 and then EtOH gave 2.2 g.

1-phenyl-3-methyl-4-hydroxy-5-benzyl-6-oxo-1,6-dihydropyrano[2,3]pyrazole, m. $226-7^\circ$ [dioxane or $(\text{Cl}_2\text{CH})_2$]. Benzosuberone (2.5 g.) and 9 g. I heated 1 hr. at $260-70^\circ$ and the crude product rubbed with petr. ether gave 4.4 g. 3-benzyl-4-hydroxy-2-oxobenzo[a]pyrano [2,3-b]cycloheptadiene (II), m. 231° (EtOAc, EtOH, dioxane, or PhCl). II (1.6 g.) and 3.2 g. AlCl_3 heated 10 min. at 140° , the mixture decomposed at 0° with dilute HCl, and the crude product repptd. from NaOH with HCl gave 1.1 g. corresponding debenzylated product, m. $196-7^\circ$ (PhCl or xylene). α -Tetralone (1.5 g.) and 2.4 g. I heated 30 min. at 255° and the crude product rubbed with C_6H_6 gave 0.95 g. 3-benzyl-4-hydroxy-5,6-dihydro-7,8-benzocoumarin (III), m. $222-3^\circ$ (PhCl or AcOH). III (0.43 g.) and 0.7 g. AlCl_3 heated at 150° and the mixture decomposed with dilute HCl gave 0.2 g. 4-hydroxy-7,8-benzocoumarin, m. 276° (dilute EtOH, PhCl, or AmOAc). 1,4-Cyclohexanedione (0.2 g.) and 2.4 g. I heated 20 min. at 260° , cooled, rubbed with C_6H_6 , and recrystd. from PhCH_2OH , PhNO_2 , or

p-cresol

gave 0.4 g.

4,8-dihydroxy-3,7-dibenzyl-2,6-dioxo-1,5-dioxo-1,2,5,6,9,10-hexahydroanthracene, m. 365° (decomposition); diacetate m. $256-7^\circ$ (xylene or PhCl). Coumaranone (0.6 g.) and 2.4 g. I heated 10 min. at 255° and the product rubbed with C_6H_6 gave 0.9 g.

3-benzyl-4-hydroxy-2-oxopyrano[3,2-b]benzofuran, m. $245-7^\circ$ (PhNO_2 , AcOH, or Tetralin). 3-Hydroxythianaphthene and 2.9 g. I heated 10 min. at

255° and the product rubbed with C_6H_6 gave 1.3 g.

3-benzyl-4-hydroxy-2-oxopyrano [3,2-b]thianaphthene, m. 247° (EtOH, AcOH, or PhNO_2). 1-Hydrindone (0.65 g.) and 2.4 g. I heated 45 min. at 250° and the product (0.9 g.) rubbed with C_6H_6 gave

3-benzyl-4-hydroxy-2-oxoindeno[1,2-b]pyran (IV), m. 273° (PhNO_2).

IV (0.96 g.) and 1.35 g. AlCl_3 heated 7 min. at $140-50^\circ$, the product repptd. from aqueous NaOH with HCl, and crystallized from dioxane- H_2O with

C gave 0.4 g. 4-hydroxy-2-oxoindeno[1,2-b]pyran, m. $244-5^\circ$

(decomposition). Flavanone (1.12 g.) and 2.9 g. I heated 1 hr. at $270-80^\circ$, allowed to stand 1 day, and rubbed with 1:1

C_6H_6 -cyclohexane gave 0.5 g.

1-hydroxy-2-benzyl-3-oxo-10-phenyl-4,9-dioxo-

3,4,9,10-tetrahydrophenanthrene, m. 218° (EtOH, PhCl, or AcOH);

10/552,459

monoacetate m. 204.5° (AcOH). peri-Naphthindandione (0.36 g.) and 1.2 g. I heated 35 min. at 250° gave 0.6 g. 8-hydroxy-9-benzyl-7,10-dioxo-11-oxa-10,11-dihydrobenzanthrene, m. 256-7° [dioxane, (Cl₂CH)₂, or PhNO₂]. BzCH₂ (1.12 g.) and 2.9 g. I heated 1 hr. at 270°, the 2,4-Cl₂C₆H₃OH distilled, and the product rubbed with 1:1 C₆H₆-cyclohexane gave 0.4 g. 3-benzyl-4-hydroxy-6-phenyl-2-pyrone, m. 251° (EtOH or AcOH). Acetylacetone monoanil (1.8 g.) and 4.8 g. I heated 12 min. at 260° gave 1.9 g. O.CO.C(CH₂Ph):C(OH).C(CMe:NPh):C Me, m. 247-8° [(Cl₂CH)₂-EtOH or PhNO₂].

=> log y

COST IN U.S. DOLLARS

SINCE FILE

TOTAL

ENTRY

SESSION

FULL ESTIMATED COST

85.26

257.57

DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)

SINCE FILE

TOTAL

ENTRY

SESSION

CA SUBSCRIBER PRICE

-12.48

-12.48

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